1,4-Benzoquinone
106-51-4 | DTXSID6020145

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 190 °C

Global applicability domain: Inside

Local applicability domain index: 6.68e-01

Confidence level: 7.33e-01

Nearest Neighbors from the Training Set

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Benzaldehyde
Measured: 179
Predicted: 195

Image not found

4-Methylbenzaldehyde
Measured: 205
Predicted: 200

Image not found

2-Tolualdehyde
Measured: 200
Predicted: 200

Image not found

Benzaldehyde, 3-methyl-
Measured: 199
Predicted: 200

Image not found

2-Furancarbonyl chloride
Measured: 173
Predicted: 208